Modeling Materials in Reactor Environments

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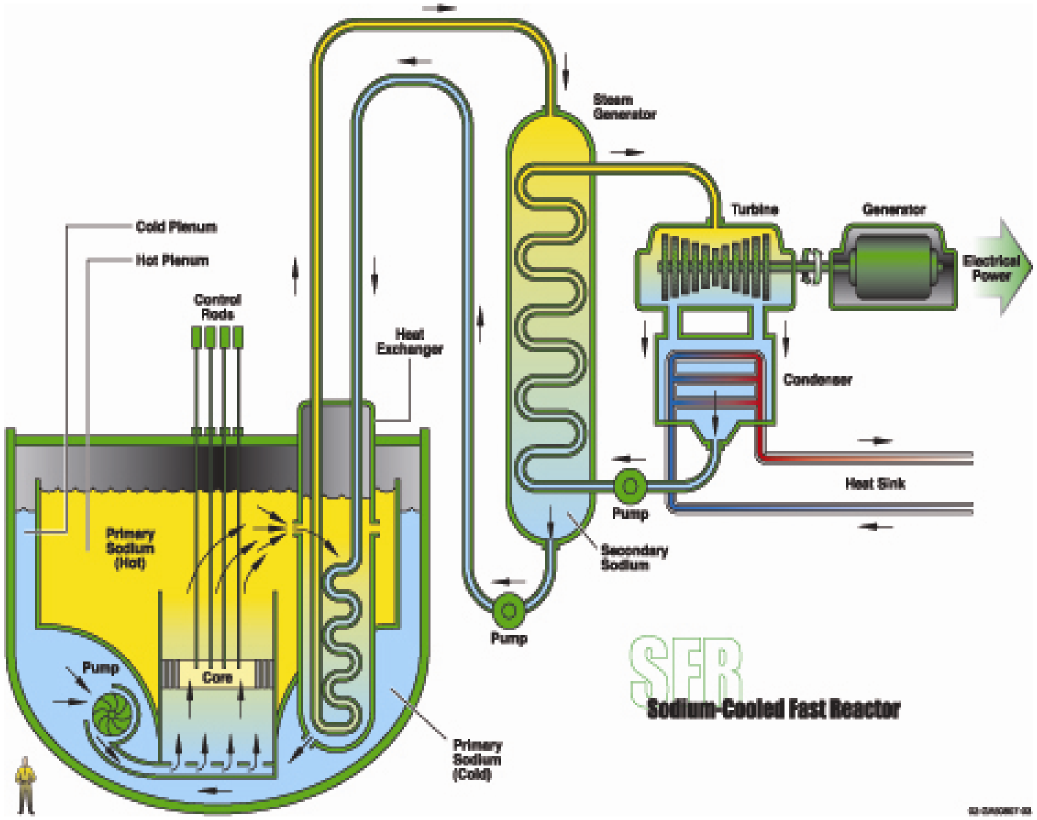
This work was performed under the auspices of the U.S. Department of Energy by University of California Lawrence Livermore National Laboratory under contract No. W-7405-Eng-48.

DOE considering building a sodium-cooled fast reactor as part of new US nuclear power infrastructure

- **Advanced fuel cycle including recycling and reprocessing**
  - **Will reduce fuel cycle waste stream by orders of magnitude**
  - **Burning Pu and minor actinides will mitigate proliferatiuon concerns**



- **SFR Operating Conditions**
  - Output Power 350-1500 MWe
  - Fast 1MeV neutron fluxes
  - Outlet Temperature 550°C
  - Low core pressure ~1 atm
  - Fuel contains significant amounts of Pu, Am, Cm, Np
  - Fuel pins withstand 20% burnup

Material Properties of Fuel Pins Limit the Performance of Sodium-Cooled Fast Reactors

Efficiency in the development, design, and licensing phases are essential to success

- **Rapid prototyping can reduce costs and schedules**
  - **Full reactor system**
  - **Fuel cycle**
  - **Major structural components and systems**
  - **Secondary system**
- **Reliability in predicting cost, schedule, and regulatory action is essential**
  - **Fuel supply**
  - **Reactor design**
  - **Repository design and availability**
  - **National and international context**
- **We must pick the "sweet spots" for investment to maximize impact on the most important issues**

Materials modeling and simulation will cut time to fuel assembly certification in two ways

- **Provide screening tools to narrow the parameter space that must be experimentally investigated**
  - **Range of fuel chemical compositions**
  - **High confidence extrapolations of fuel element performance to large irradiation doses**

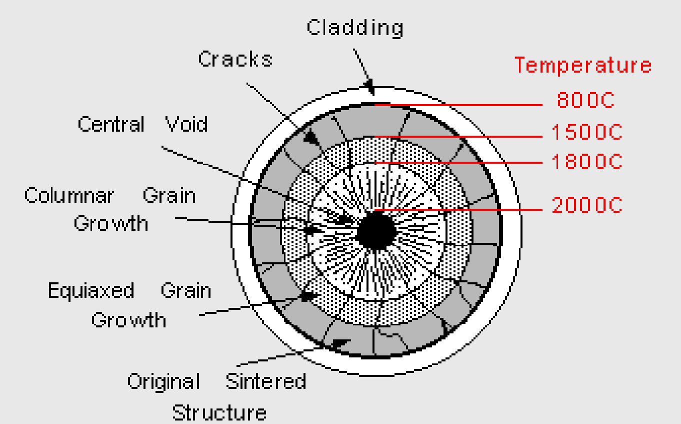
- **Performance models coupled with “neutronics” packages will create robust fuel pin design software**
  - **Thermo-mechanical performance of a fuel pin in service conditions**
  - **Identify life limiting mechanisms and test solutions**

There are currently no active test reactors to irradiate samples for a purely experimental campaign

Materials limit the performance of the reactor and determine fuel pin life limits

– Fuel

- **Dimensional Stability with Evolving Fuel Chemistry**
  - Swelling due to fission products and transmutant elements
  - Swelling due to irradiation damage and Helium retention
  - Volume change to due element segregation and phase change
  - Changes to coefficients of thermal expansion
- **Heat Transfer with Evolving Fuel Chemistry**
  - Changes in Thermal Conductivity
  - Changes in Heat Generation
- **Mechanical Integrity**
  - Development of Cracks
  - Changes in Mechanical Properties
- **Neutron Cross-Section**
- **Helium and Fission Gas Release**



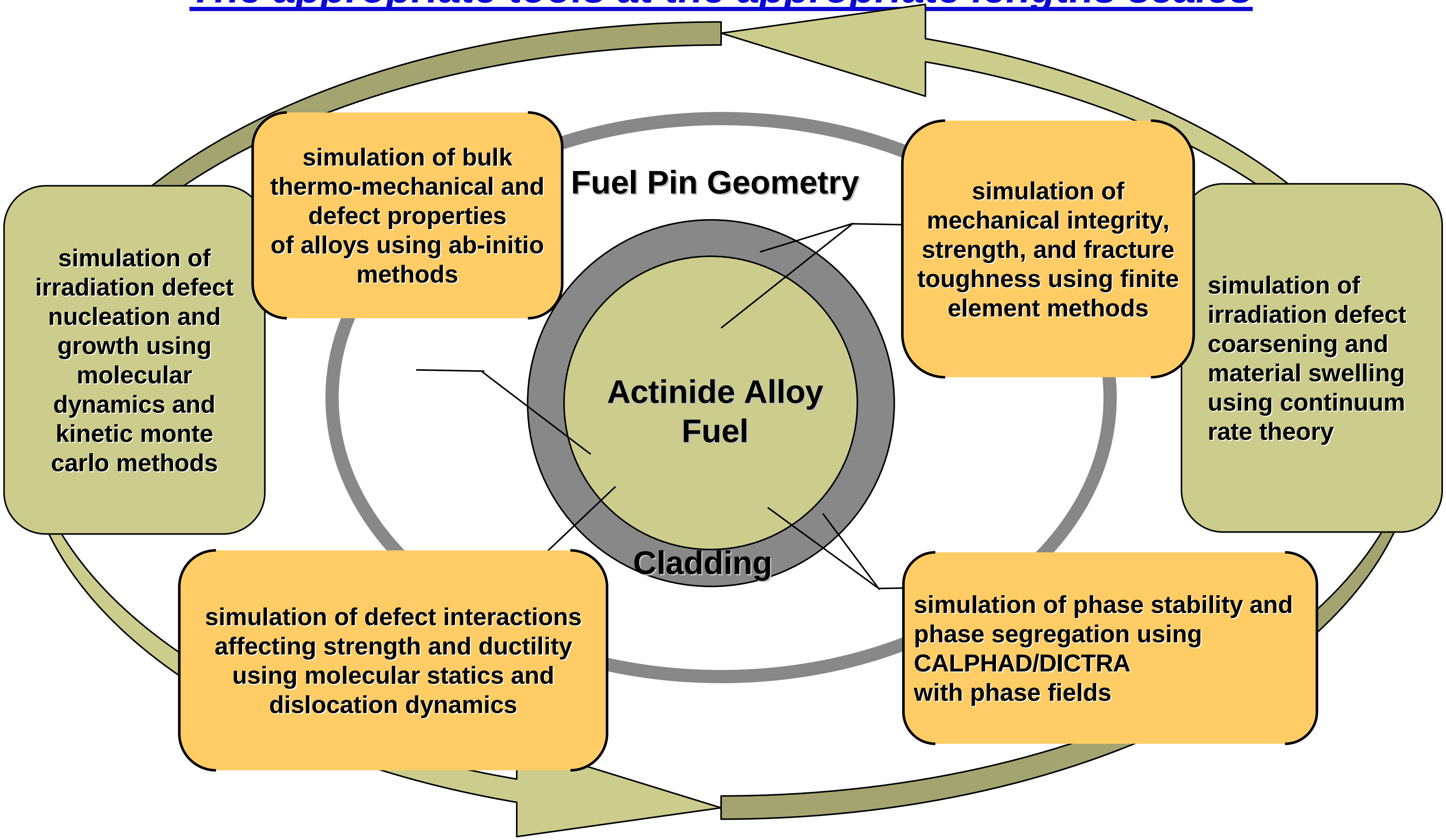
M.A Speer, UCB

– Cladding

- **Thermo-Mechanical Properties and Dimensional Stability**
  - Swelling due to irradiation damage
  - Alloy segregation
  - Creep due to high temperature and pressure buildup
  - Changes in ductility and fracture toughness due to irradiation damage
- **Corrosion**
  - Fuel/Cladding interface degradation
  - Fuel/Coolant interface degradation

LLNL has the experience to integrate a unique tool set and focus on reactor fuel issues

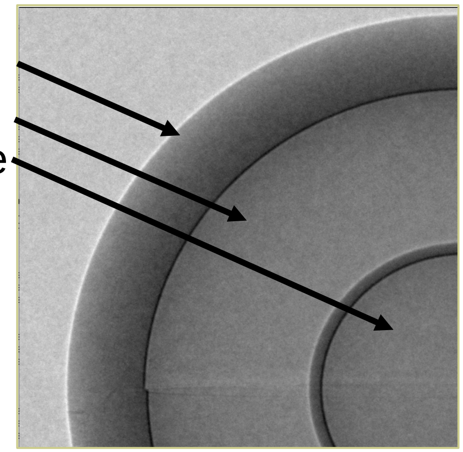
The appropriate tools at the appropriate lengths scales



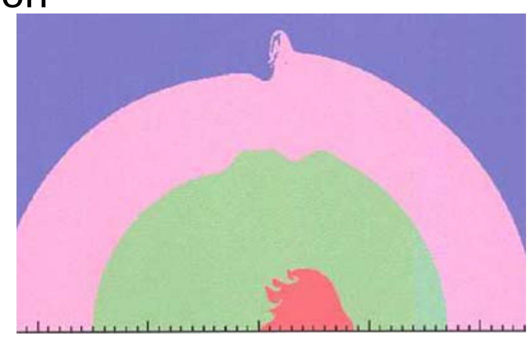
LLNL Advanced Scientific Computing has been applied to complex issues in materials structure and performance

We predicted the performance of a Double shell laser target

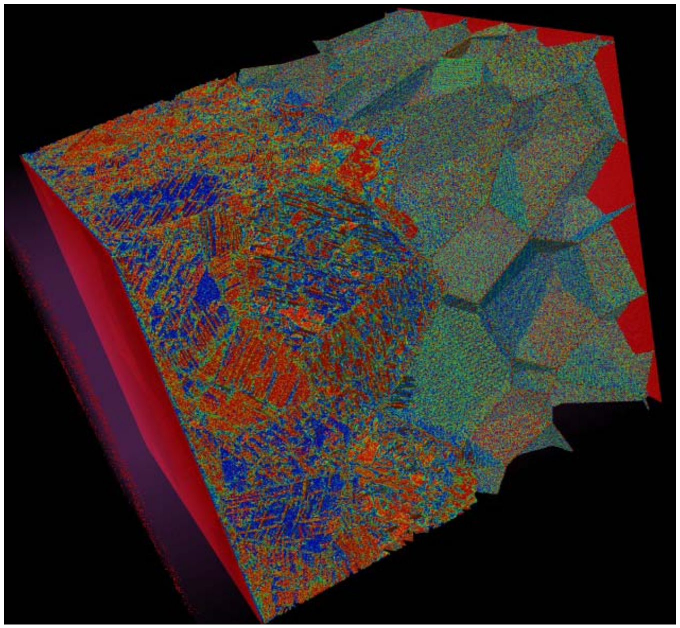
50 μm plastic ablator
50 mg/cc SiO_2 layer
200 μm glass capsule



1.5 μm flaw led to major yield reduction



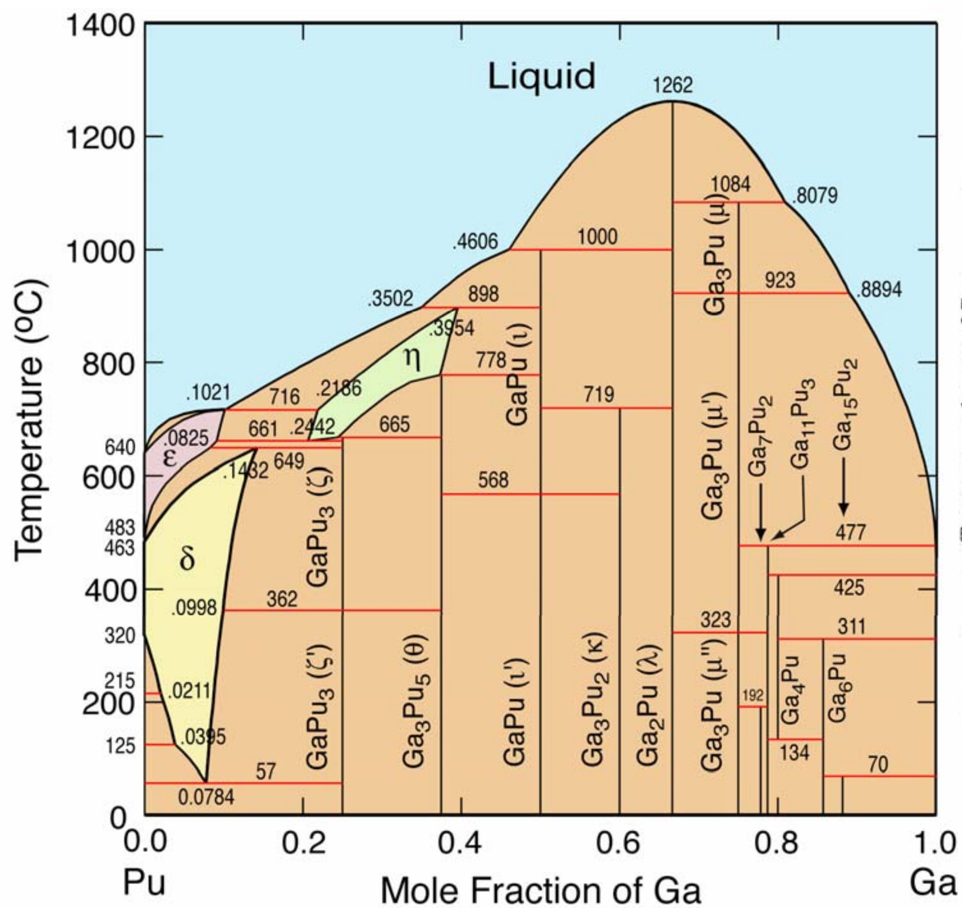
Radius (mm)



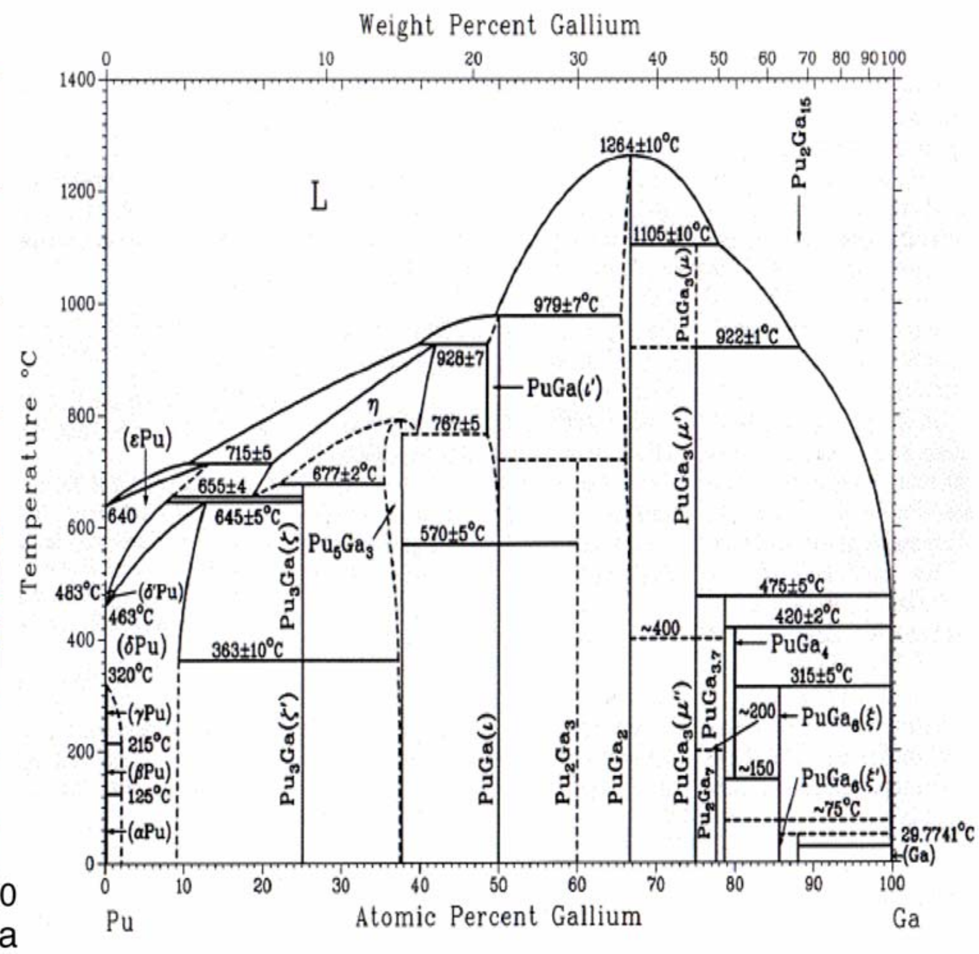
We developed fundamental understanding of nanograined materials' strength in laser-shock dynamic experiments

CALPHAD Thermodynamic database is extended to asses the phase stability of plutonium alloys

CALPHAD Assessment of Pu-Ga Phase Diagram



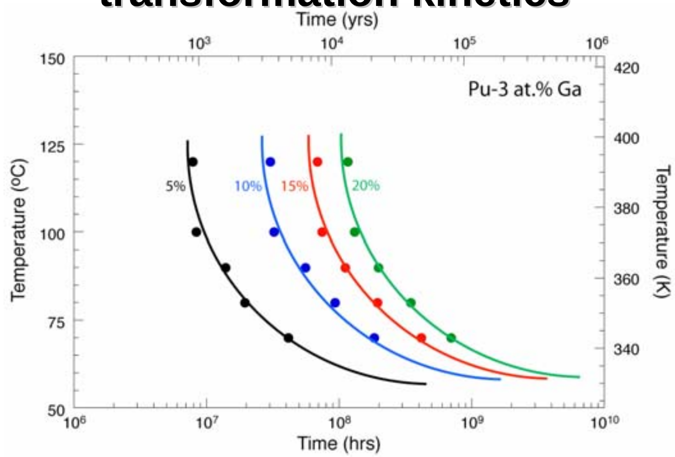
Experimental Assessment of Pu-Ga Phase Diagram (Ellinger "US" version)



CALPHAD combined with DICTRA and phase field modeling can predict phase segregation

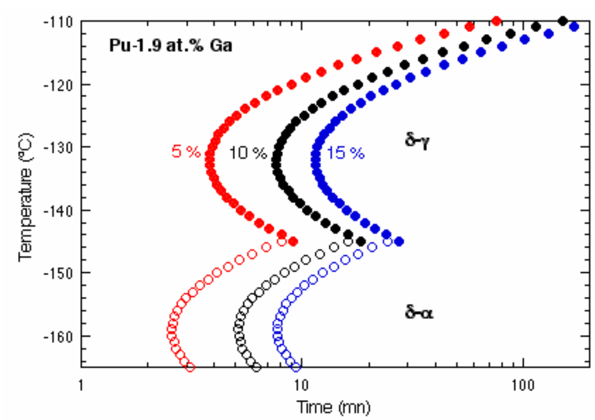
DICTRA provides phase transformation kinetics

Diffusional



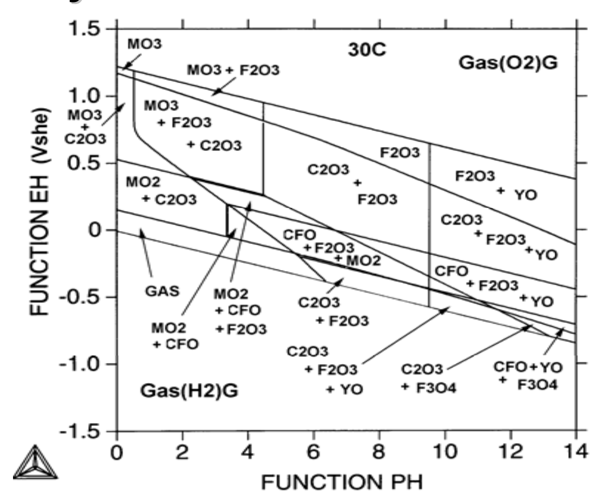
Simulated Kinetics of δ to α phase transition

Martensitic



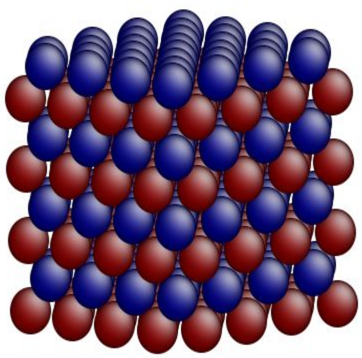
Microstructural evolution of complex alloys with phase field methods

Pourbaix diagram analysis of material reactivity in corrosive environments

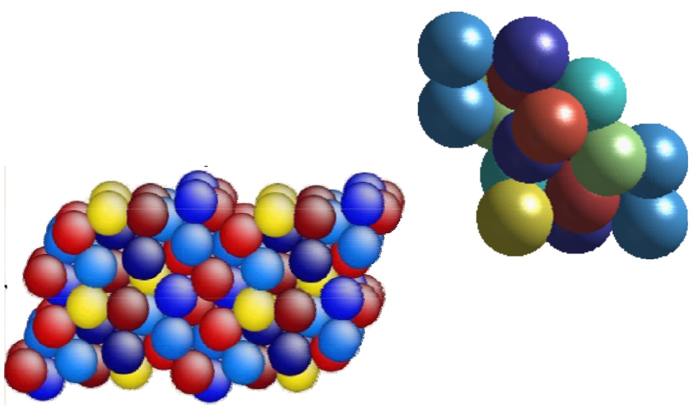


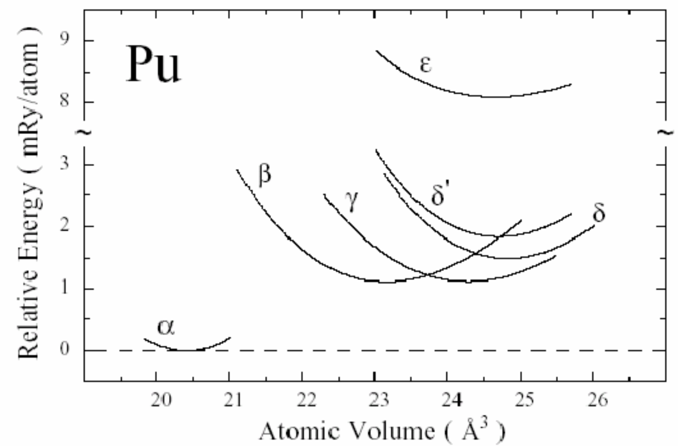
Ab Initio methods have been used to calculate defect & bulk physical properties of actinides

Ga stabilization of δ-phase Pu

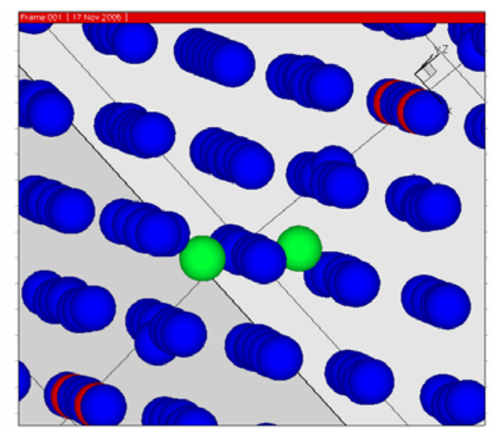


Calculation of lattice site specific atomic energy in α- and β- phases of Pu





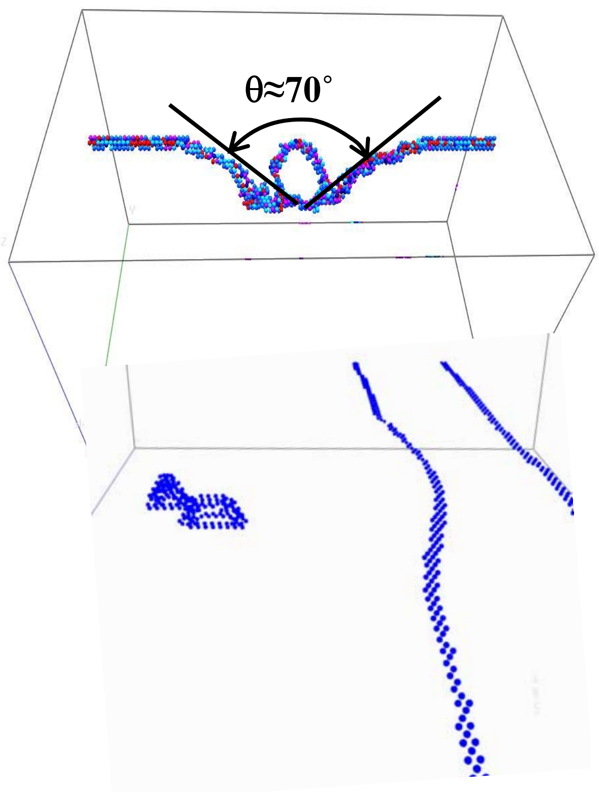
Calculation of atomic volumes in Pu phases



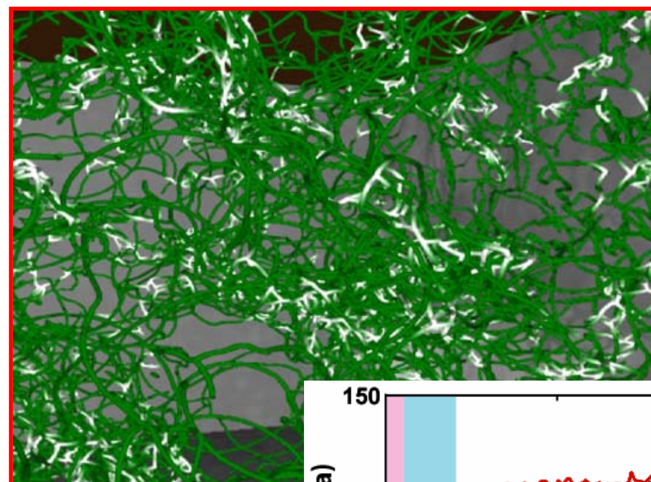
Calculation of formation energy of interstitials in Ga-stabilized Pu: 0.8 eV - 1.8 eV

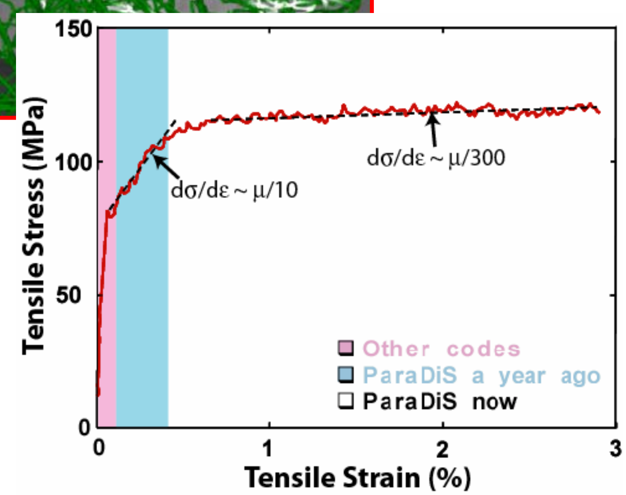
Simulations of defect interactions uncover the origins of strength and ductility of metals

Molecular statics simulations detail the interactions of dislocations with irradiation induced defects



Dislocation dynamics simulations uncover the nature of dislocation multiplication and work hardening

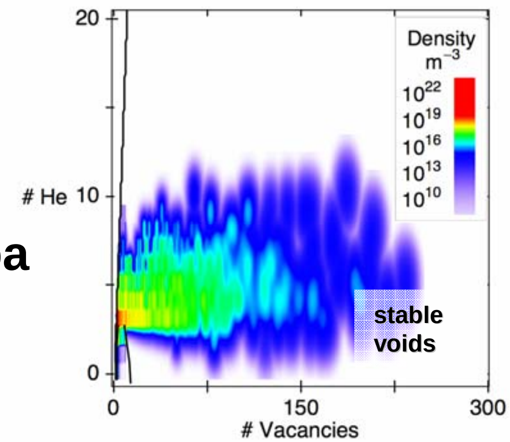




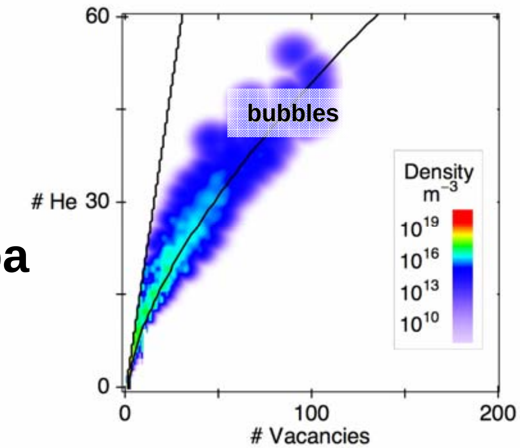
Kinetic rate theory can predict the swelling rate of fuel cladding due to the accumulation of irradiation damage

Defect clusters separate into a mix of equilibrium bubbles and stable/unstable voids depending on radiation environment

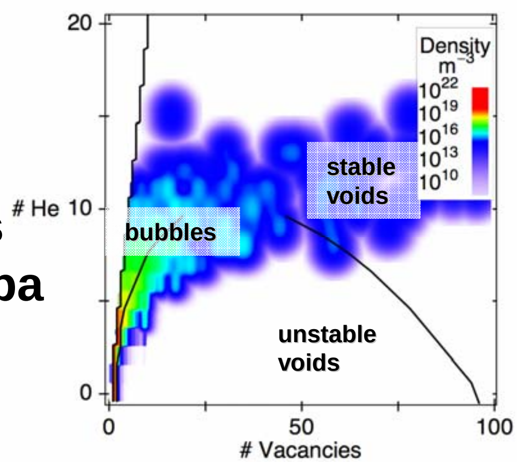
300 C
10^{-6} dpa/s
64×10^{-3} dpa



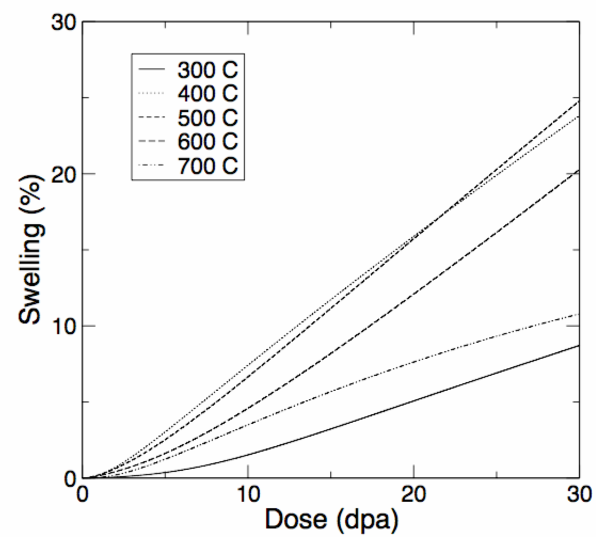
700 C
10^{-6} dpa/s
64×10^{-3} dpa



500 C
10^{-6} dpa/s
16×10^{-3} dpa



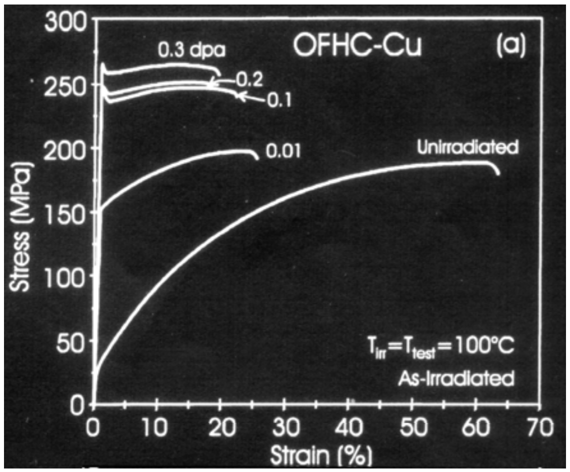
Swelling predictions due to void/bubble distributions



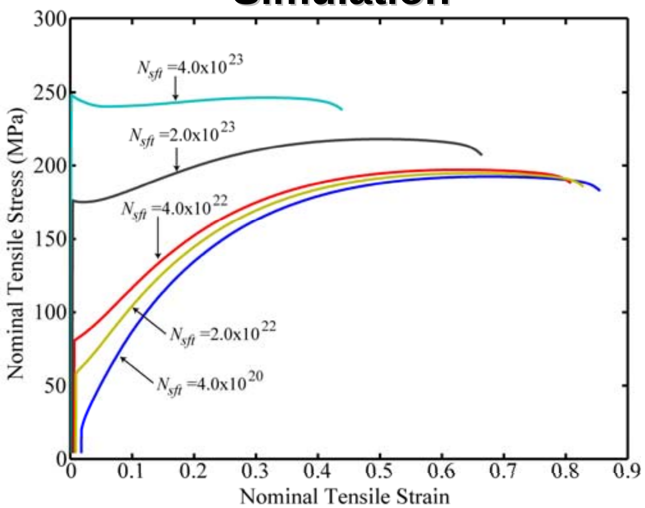
Microstructural information is used to determine macroscopic mechanical behavior of irradiated materials

Experiment

B. Singh et al., (2001), *J. Nucl. Mat.*, 299, 205



Simulation



Fracture and strength models can be combined to simulate dynamic failure and fragmentation

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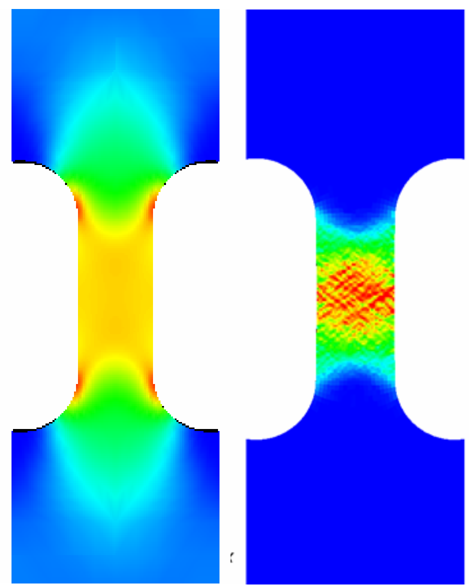
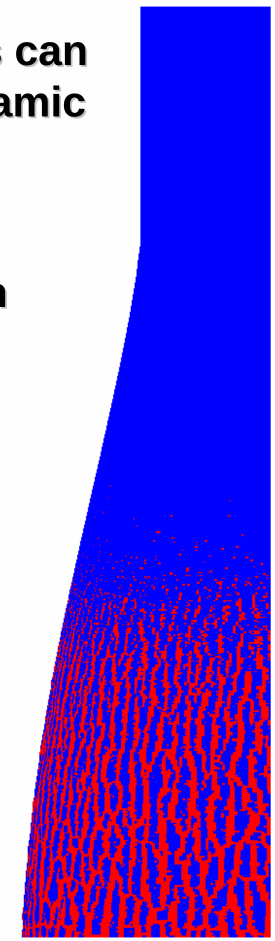
Flow localization of irradiation damaged materials



unirradiated **irradiated**



Materials modeling and simulation of fuel pin performance will require code development

- Simulation tools discussed are generic tools that can be applied to solve materials issues in fast reactor environments
  - Current simulation capabilities are not focused on fuel and cladding performance – cannot just simply run existing codes with a change in constants
  - Devil is in the Details – Material Specificity
    - ab initio handling of f-electrons in solids
    - CALPHAD thermodynamic database is incomplete for actinides
    - Molecular potentials for actinides
    - Dislocation and irradiation defect reactions not understood
    - Strength modeling of systems with multiple phases
- To build simulations capabilities effective in modeling fuel pin performance significant investments must be made in developing and extending of these tools to the problems of interest

Materials modeling and simulation can accelerate certification of nuclear reactor fuel elements

- **Materials modeling and simulation for the stockpile stewardship mission has led to understanding materials performance determined by physics at disparate length scales**
- **Role of modeling and simulation will be to:**
  - **Provide guidance to narrow the experimental space that is investigated**
  - **Provide insight with which to meaningfully interpret experimental findings**
  - **Make credible extrapolations and predictions of fuel element performance to lifetime limits and accident scenarios for design purposes**

all of which lead to shorter development times for fuel chemistry selection and certification and fuel pin design